CASE WESTERN RESERVE UNIVERSITY EST. 1826

An Investigation of Hydrocarbon Flames using Probe Sampling and GC/MS

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Presentation Outline

- Background
  - Fuels
  - Fundamentals of Gas Chromatography and Mass Spectrometry
- Experimental Apparatus and Procedure
  - Shimadzu GCMS-QP2010 Plus
  - Analysis Techniques
- Results
  - Jet A, JP8, S-8 Results
  - Fuel Comparisons
- Future Work
  - Extend work to flame studies
- Acknowledgements

Background

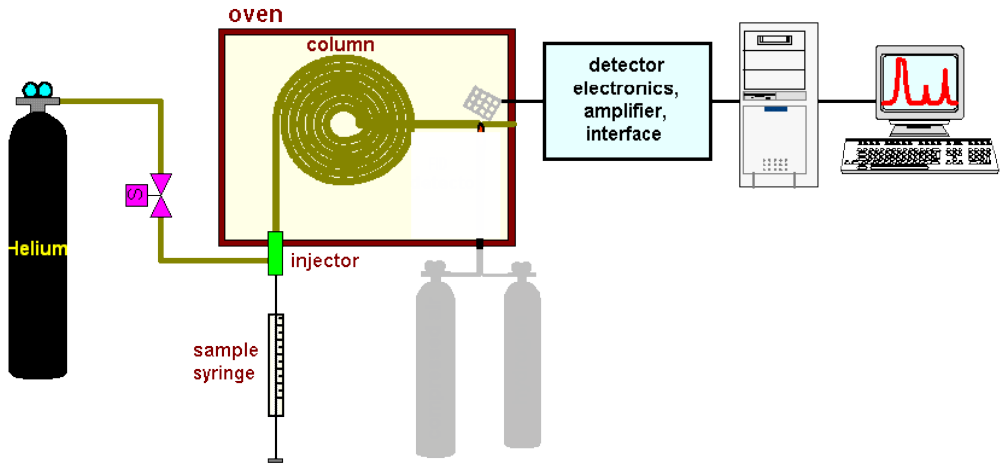
- Modern hydrocarbon fuels are complex
- Reaction kinetics of heavy hydrocarbons (>C6) are not well understood
- Experimental work requires less complex mixtures
- When we understand how a fuel burns, we can create better alternatives

Background

- GC is good at separating mixtures, not at determining components
- MS is good at determining single components, but not mixtures
- Combining GC and MS allows “best of both worlds” analysis

Background

- Fundamental Operation of a Gas Chromatograph
  - Primary Pieces



  - Column separates sample mixtures
  - Mixture components are slowed at different rates by the column

Background

- Fundamental Operation of a Mass Spectrometer
  - Primary Pieces

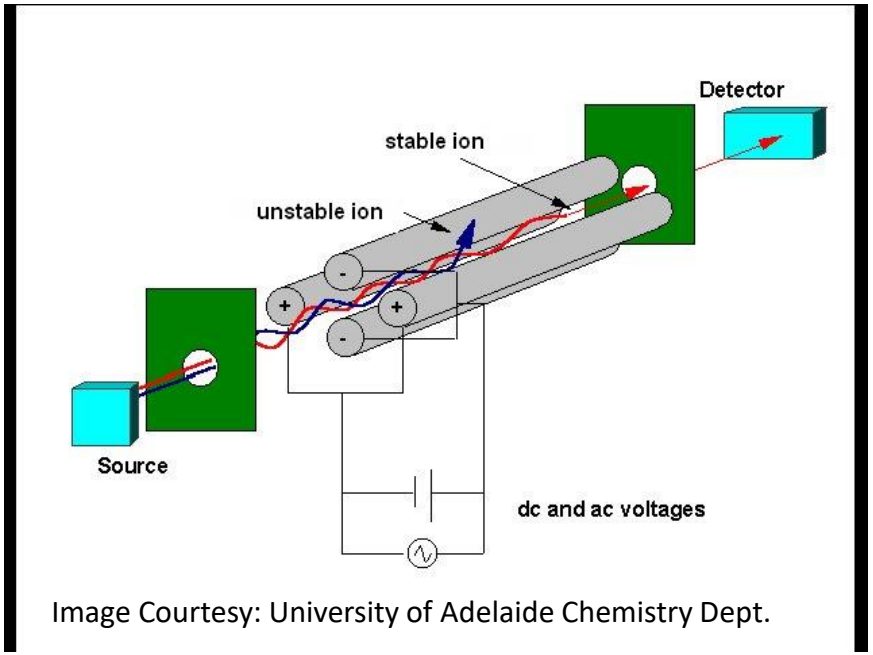


Image Courtesy: University of Adelaide Chemistry Dept.

  - Source creates electrically charged particles
  - Varying voltages filter ions by weight

Apparatus

- Shimadzu GCMS-QP2010Plus

Image courtesy: http://ssi.shimadzu.com

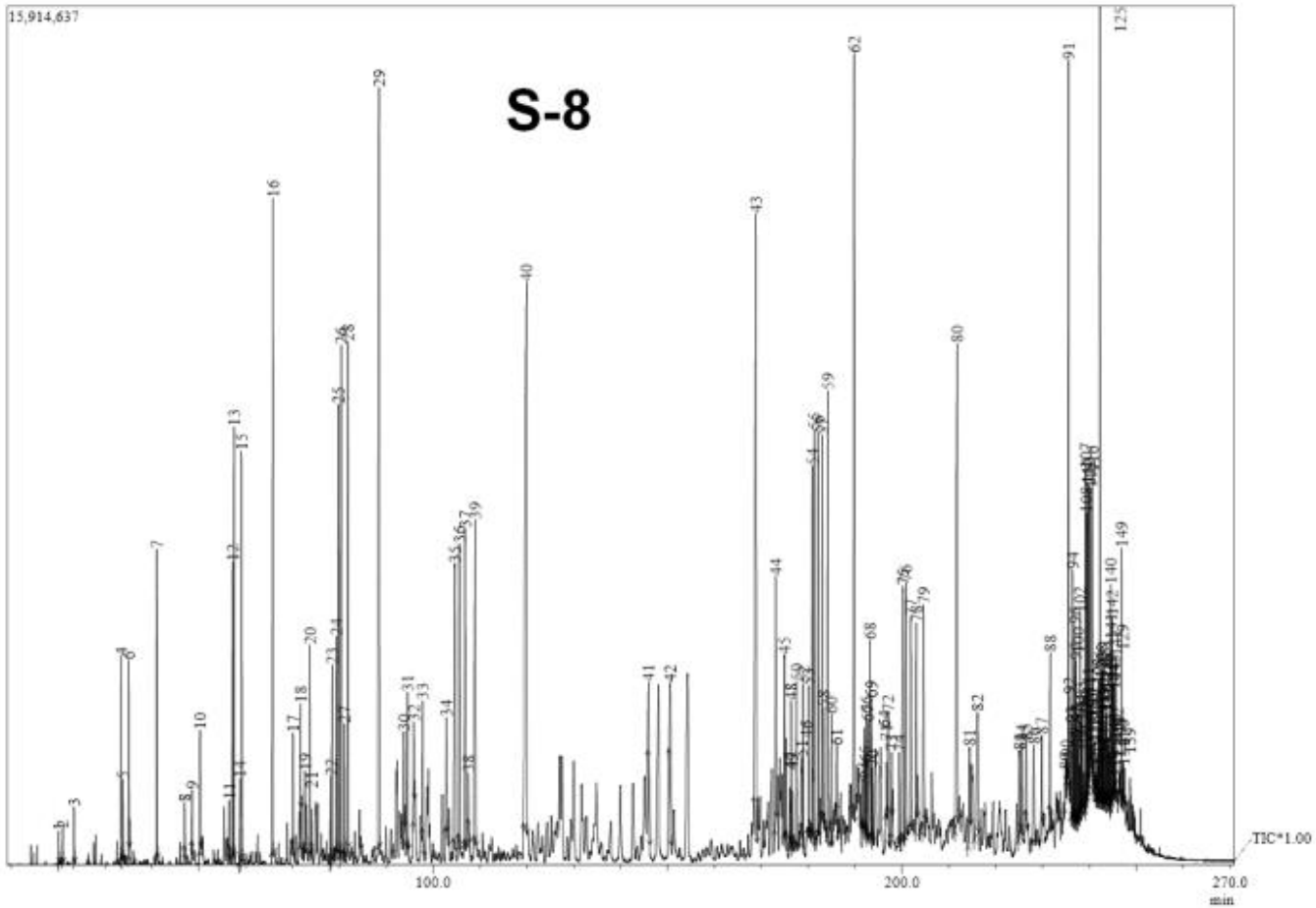
Procedure

- Analysis using GC/MS is an empirical procedure
- Temperature programs are optimized for different fuels and columns

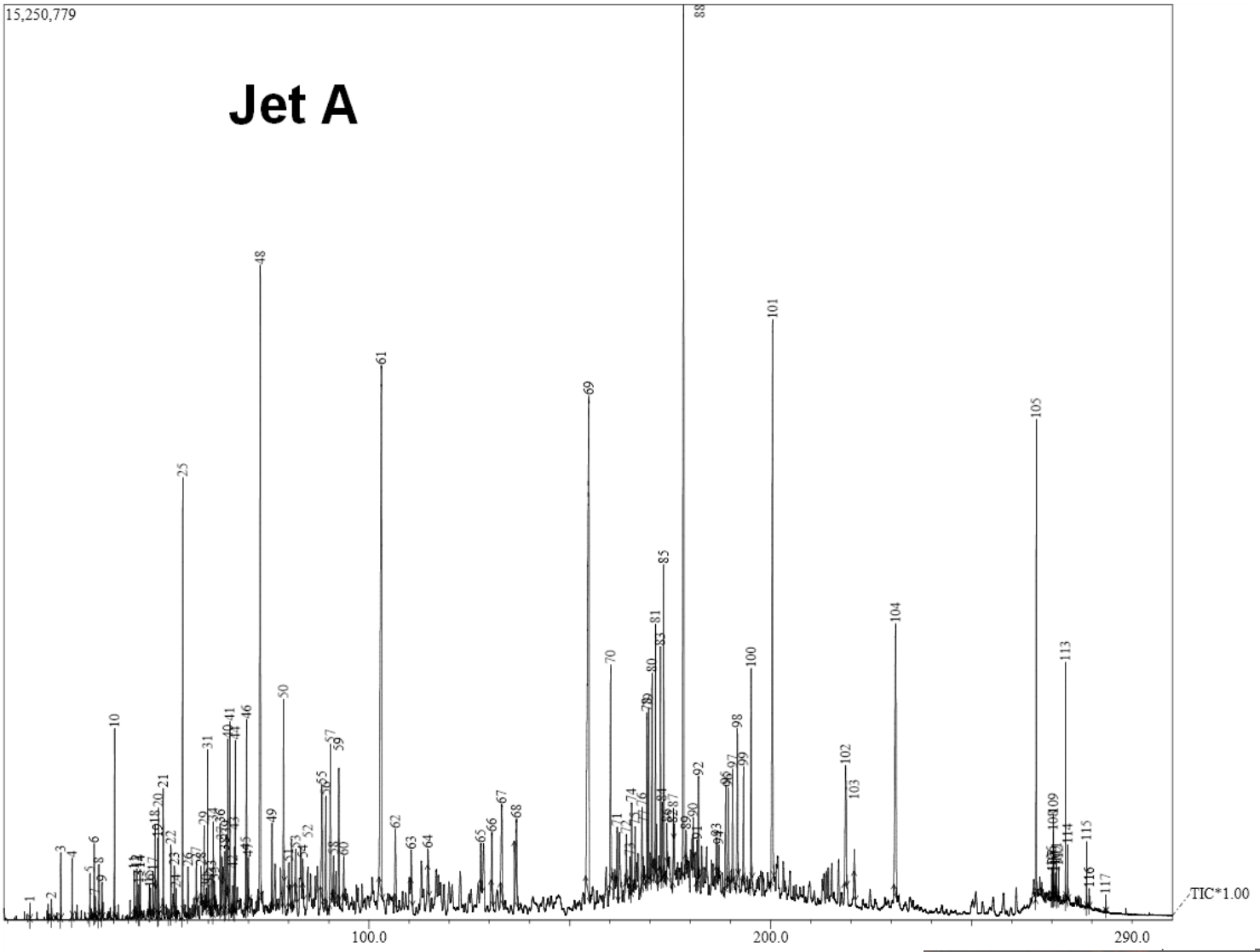
Results

Name	Jet A	JP8	S-8
# of Peaks Identified	117	141	149
Primary Species:	Dodecane	Decane	Octane
	Hexadecane	Dodecane	Nonane
	Decane	Tridecane	Decane
	Octane	Cyclohexane	Undecane
	Cyclohexane	Benzene	Dodecane
	Benzene	Benzene Isomers	
	Benzene Isomers	Non-Hydrocarbon Additives	

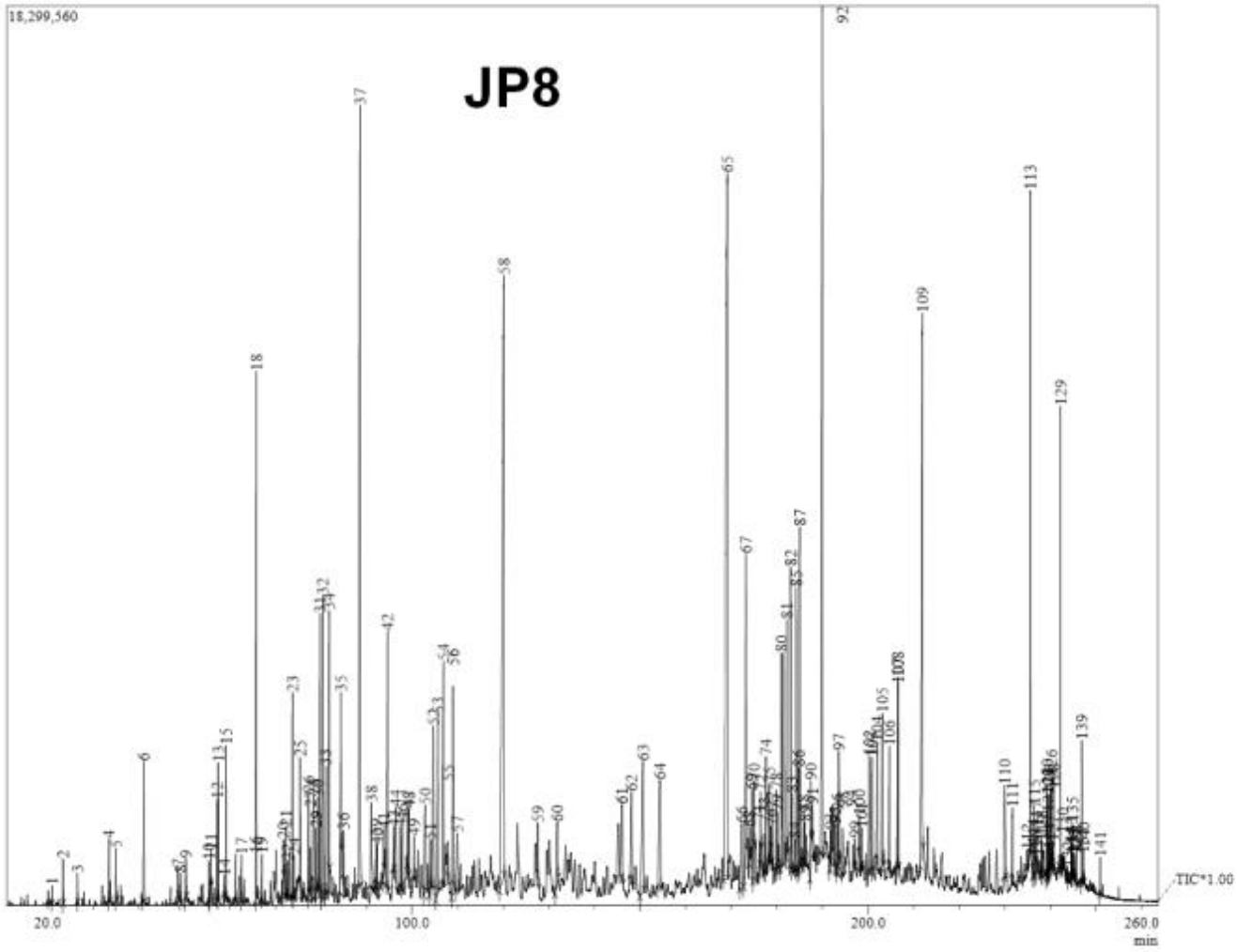
Results



Results



Results

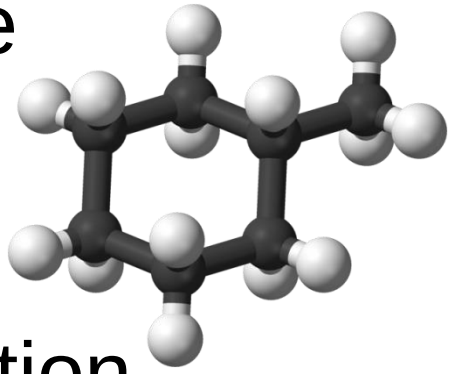


Results

- Comparison between fuels:
  - S-8 tends to have shorter chains
  - S-8 contains more isomers of methyl groups attached to the chain
  - Jet A and JP8 have similar weights
  - JP8 contains a significant number of ring-shaped molecules (cyclohexane, benzene)

Future Work

- Help Dr. Gaurav Mittal complete methylcyclohexane study



- Continue to investigate combustion chemistry of real jet fuels and their surrogates
  - Improve fundamental understanding of oxidation reactions of pure fuel components
  - Characterize chemical interactions of fuel blends

Acknowledgments

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